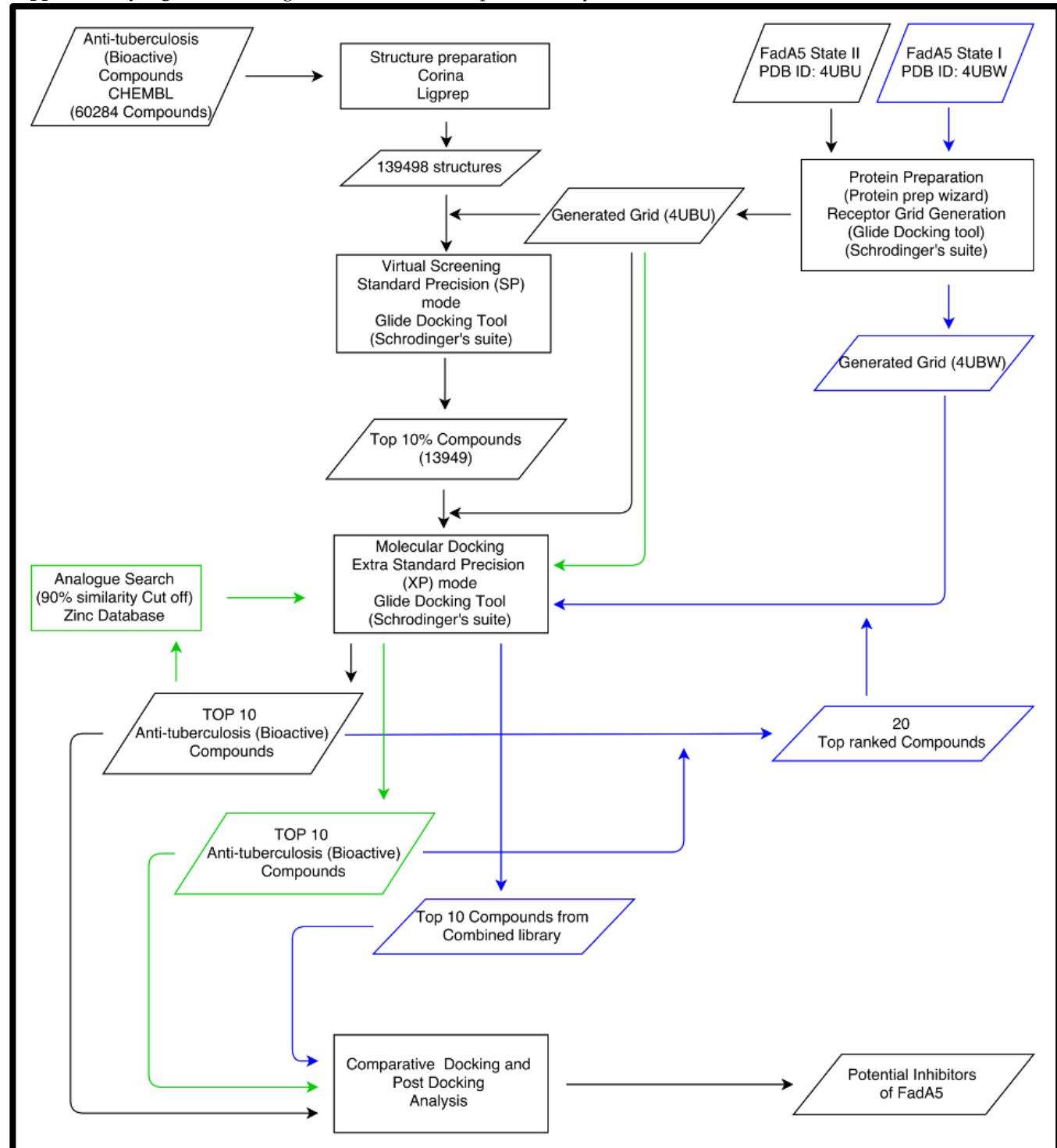
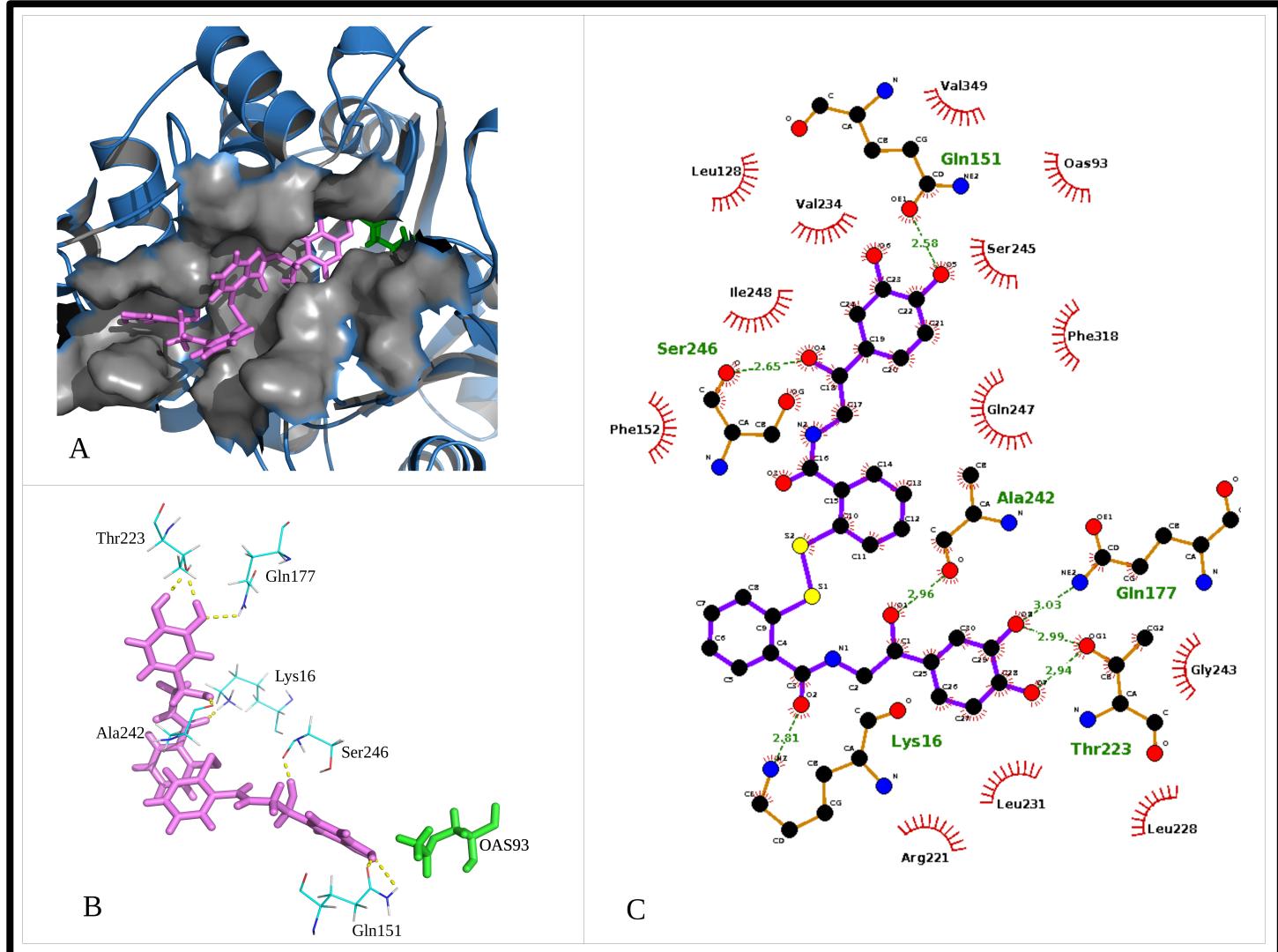


Supplementary data:

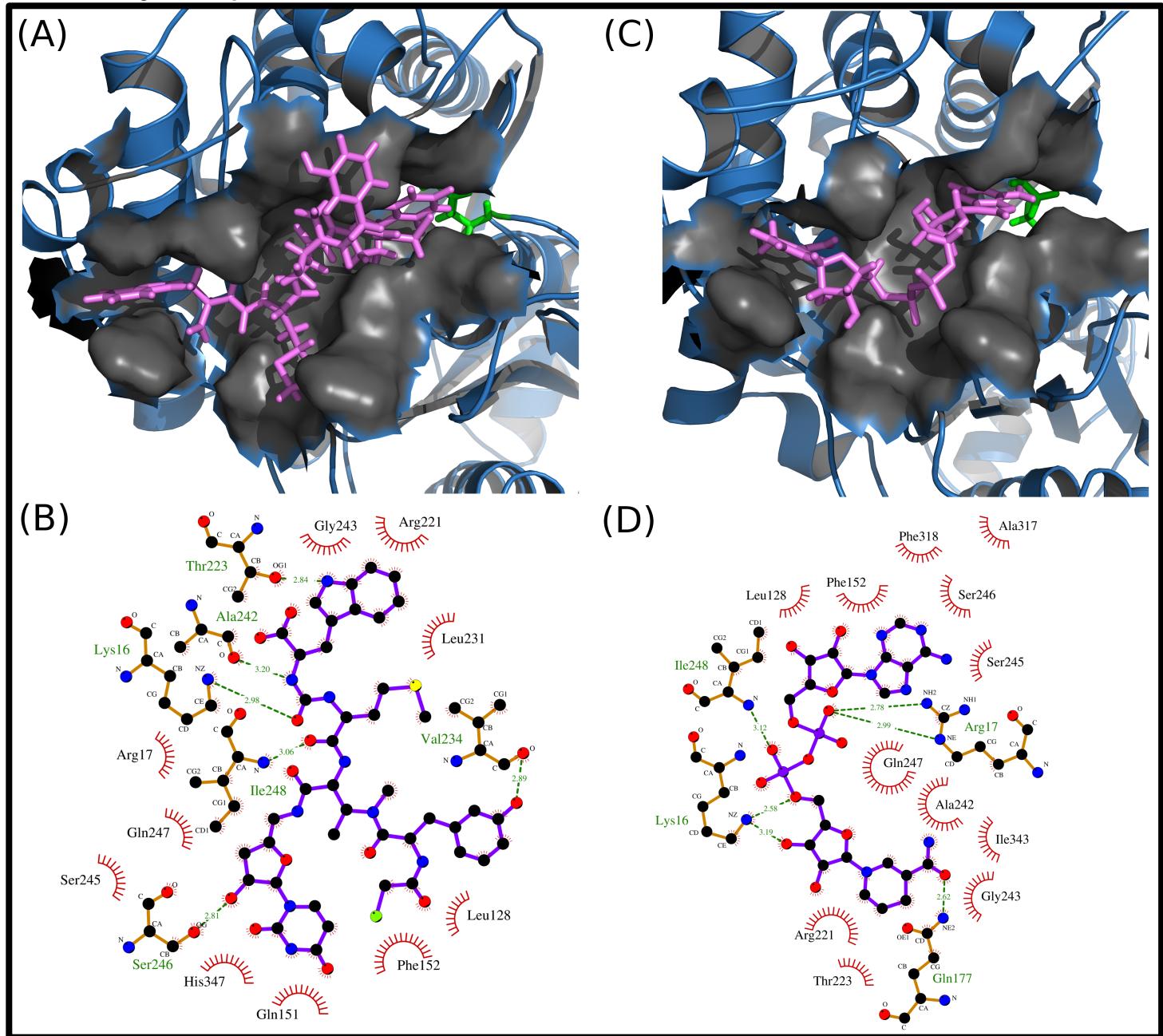
Supplementary Figure 1: Docking workflow used in the present study.



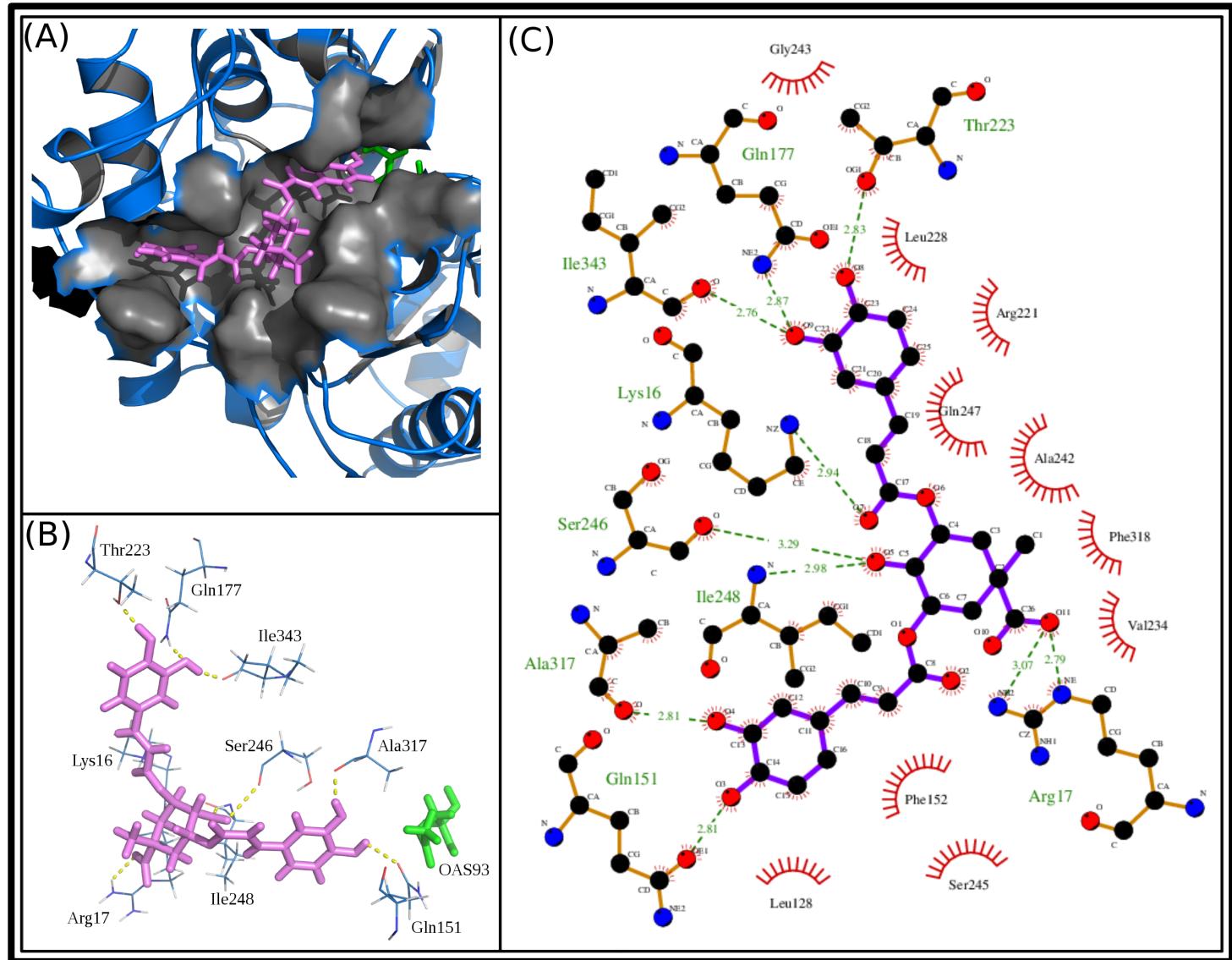
Supplementary Figure 2: (A) Compound C1 bound to FadA5 state II, (B) hydrogen bonding interaction of C1 and active site amino acid residues and (C) ligand interaction profile of C1 in the binding pocket. Legends of protein ligand interactions are given in **Figure 1**.



Supplementary Figure 3: (A) Compound C8 bound to FadA5 state II, (B) 2D interaction profile of C8 in the binding pocket, (C) Compound Z5 bound to FadA5 state II and (D) 2D interaction profile of Z5 in the binding pocket. Legends of protein ligand interactions are given in **Figure 1**.



Supplementary Figure 4: (A) Compound Z2 bound to FadA5 state II, (B) hydrogen bonding interaction of Z2 and active site amino acid residues and (C) ligand interaction profile of Z2 in the binding pocket. Legends of protein ligand interactions are given in **Figure 1**.



Supplementary Table 1: Top ranking compounds against FadA5 state II structure from virtual screening of known anti-tuberculosis compounds (ChEMBL bio-assay) and analogues compounds (ZINC database).

FadA5 state II - ChEMBL				FadA5 state II - ZINC			
CID	IUPAC NAME (CHEMBL ID)	G-Score (Kcal/mol)	X-score (Kcal/Mol)	CID	IUPAC NAME (ZINCdatabase ID)	G-Score (Kcal/mol)	X-score (Kcal/Mol)
C1	(CHEMBL296650)	-12.252	-9.92	Z1	(ZINC86864386)	-12.626	-9.44
C2	(CHEMBL2024335)	-12.224	-9.10	Z2	(ZINC39351841)	-12.483	-9.81
C3	(CHEMBL250087)	-11.409	-8.46	Z3	(ZINC60392740)	-12.325	-8.46
C4	(CHEMBL2024340)	-11.405	-9.13	Z4	(ZINC03919243)	-12.198	-9.81
C5	(CHEMBL82570)	-11.065	-9.39	Z5	(ZINC60392741)	-12.012	-8.46
C6	(CHEMBL392204)	-10.957	-9.06	Z6	(ZINC77311642)	-11.817	-8.66
C7	(CHEMBL510826)	-10.867	-9.67	Z7	(ZINC38143877)	-11.732	-9.28
C8	(CHEMBL1910811)	-10.449	-10.67	Z8	(ZINC67913793)	-11.621	-9.45
C9	(CHEMBL233434)	-10.381	-8.70	Z9	(ZINC86864389)	-11.599	-9.34
C10	(CHEMBL247657)	-10.34	-10.40	Z10	(ZINC85480044)	-11.582	-8.17

CID: Compound identification number used in this paper.